

EAST UPDATE 9/910, 466

L Number	Hits	Search Text	DB	Time stamp
1	10396	(pyrimidin or pyrimidinyl or pyrimidyl) and (sulfonamide or sulfonyl or sulfonamido)	USPAT; US-PGPUB	2004/03/24 14:21
2	2167	((pyrimidin or pyrimidinyl or pyrimidyl) and (sulfonamide or sulfonyl or sulfonamido)) and alanine	USPAT; US-PGPUB	2004/03/24 14:23

09/ 910,466

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal202txn

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 09	CA/CAPLUS records now contain indexing from 1907 to the present
NEWS	4	DEC 08	INPADOC: Legal Status data reloaded
NEWS	5	SEP 29	DISSABS now available on STN
NEWS	6	OCT 10	PCTFULL: Two new display fields added
NEWS	7	OCT 21	BIOSIS file reloaded and enhanced
NEWS	8	OCT 28	BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS	9	NOV 24	MSDS-CCOHS file reloaded
NEWS	10	DEC 08	CABA reloaded with left truncation
NEWS	11	DEC 08	IMS file names changed
NEWS	12	DEC 09	Experimental property data collected by CAS now available in REGISTRY
NEWS	13	DEC 09	STN Entry Date available for display in REGISTRY and CA/CAPLUS
NEWS	14	DEC 17	DGENE: Two new display fields added
NEWS	15	DEC 18	BIOTECHNO no longer updated
NEWS	16	DEC 19	CROPU no longer updated; subscriber discount no longer available
NEWS	17	DEC 22	Additional INPI reactions and pre-1907 documents added to CAS databases
NEWS	18	DEC 22	IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
NEWS	19	DEC 22	ABI-INFORM now available on STN
NEWS	20	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
NEWS	21	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAPLUS
NEWS	22	FEB 05	German (DE) application and patent publication number format changes
NEWS	23	MAR 03	MEDLINE and LMEADLINE reloaded
NEWS	24	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	25	MAR 03	FRANCEPAT now available on STN
NEWS EXPRESS	MARCH 5 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004		
NEWS HOURS	STN Operating Hours Plus Help Desk Availability		
NEWS INTER	General Internet Information		
NEWS LOGIN	Welcome Banner and News Items		
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN		
NEWS WWW	CAS World Wide Web Site (general information)		

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 15:00:11 ON 24 MAR 2004

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:00:20 ON 24 MAR 2004

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 MAR 2004 HIGHEST RN 666817-09-0

DICTIONARY FILE UPDATES: 23 MAR 2004 HIGHEST RN 666817-09-0

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

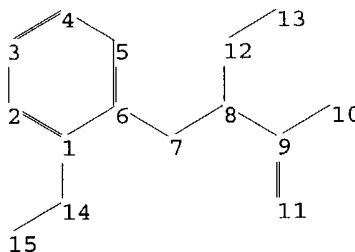
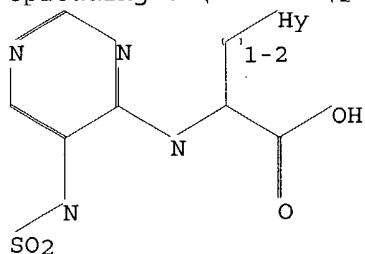
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\STNEXP4\QUERIES\09910466a.str



chain nodes :

7 8 9 10 11 12 13 14 15

ring nodes :

1 2 3 4 5 6

chain bonds :

1-14 6-7 7-8 8-9 8-12 9-10 9-11 12-13 14-15

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-14 6-7 7-8 12-13 14-15

exact bonds :

8-9 8-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-11

09/ 910,466

isolated ring systems :
containing 1 :

Match level :

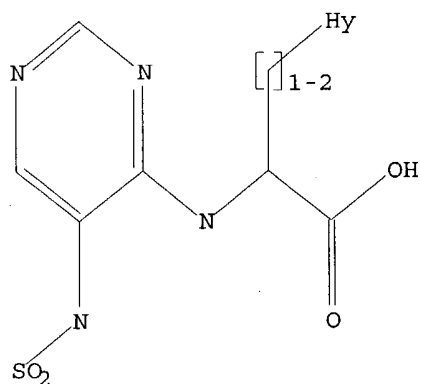
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:Atom 14:CLASS 15:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

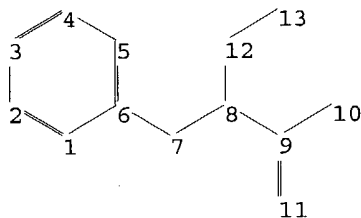
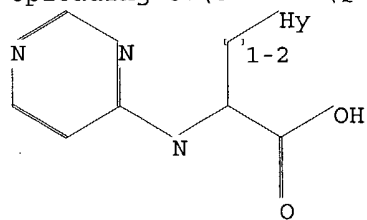
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=>

Uploading C:\STNEXP4\QUERIES\09910466b.str



chain nodes :

7 8 9 10 11 12 13

ring nodes :

1 2 3 4 5 6

chain bonds :

6-7 7-8 8-9 8-12 9-10 9-11 12-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

6-7 7-8 12-13

exact bonds :

8-9 8-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-11

isolated ring systems :

containing 1 :

09/ 910,466

Match level :

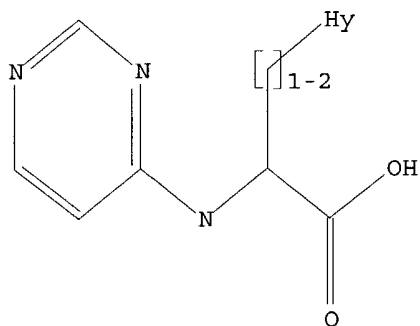
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:Atom

L2 STRUCTURE UPLOADED

=> d l2

L2 HAS NO ANSWERS

L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful

FULL SEARCH INITIATED 15:01:00 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 66 TO ITERATE

100.0% PROCESSED 66 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=> s l2 ful

FULL SEARCH INITIATED 15:01:06 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 968 TO ITERATE

100.0% PROCESSED 968 ITERATIONS

16 ANSWERS

SEARCH TIME: 00.00.01

L4 16 SEA SSS FUL L2

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

310.42

310.63

FILE 'CAPLUS' ENTERED AT 15:01:13 ON 24 MAR 2004

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FILE COVERS 1907 - 24 Mar 2004 VOL 140 ISS 13
FILE LAST UPDATED: 23 Mar 2004 (20040323/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 14

L5 13 L4

=> d 15 1- ibib abs hitstr

YOU HAVE REQUESTED DATA FROM 13 ANSWERS - CONTINUE? Y/(N):y

L5 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:319721 CAPLUS

DOCUMENT NUMBER: 138:321292

TITLE: Preparation of 2,4,5-trisubstituted pyrimidines as cyclin dependent kinase inhibitors

INVENTOR(S): Dahmann, Georg; Himmelsbach, Frank; Wittneben, Helmut; Pautsch, Alexander; Prokopowicz, Anthony S.; Krist, Bernd; Schnapp, Gisela; Steegmaier, Martin; Lenter, Martin; Schoop, Andreas; Steurer, Steffen; Spevak, Walter

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany; Boehringer Ingelheim Pharmaceuticals, Inc.; Boehringer Ingelheim International G.m.b.H.

SOURCE: PCT Int. Appl., 278 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003032997	A1	20030424	WO 2002-EP11453	20021014

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

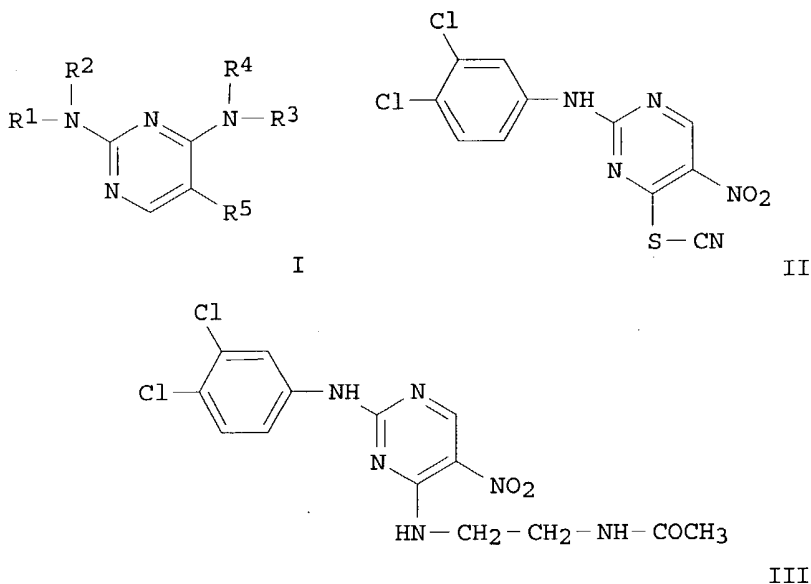
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003171359	A1	20030911	US 2002-271763	20021016
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PRIORITY APPLN. INFO.: US 2001-330145P P 20011017

OTHER SOURCE(S): MARPAT 138:321292

GI



AB Title compds. I [R1 = H, alkyl; R2 = (un)substituted alkyl; R3 = H, alkyl; R4 = (un)substituted alkyl; R5 = halo] and their pharmaceutically acceptable salts were prepared. For example, condensation of thiocyanatopyrimidine II, e.g., prepared from 3,4-dichloroaniline and 2-chloro-4-thiocyanato-5-nitropyrimidine in one step, and acetylaminioethylamine provided trisubstituted pyrimidine III in 88% yield. In CDK1/CyclinB1 kinase inhibition studies, 88-examples of compds. I exhibited IC50 values more than 100 nM. Compds. I are claimed useful for the treatment of diseases characterized by abnormal cell proliferation.

IT **514831-25-5P**, 2-(3,4-Dichlorophenylamino)-4-[(1S)-1-carboxy-2-(1H-imidazol-4-yl)ethyl]amino]-5-trifluoromethylpyrimidine
514832-15-6P, 2-(3,4-Dichlorophenylamino)-4-[(1R)-1-carboxy-2-(1H-imidazol-4-yl)ethyl]amino]-5-trifluoromethylpyrimidine
514832-70-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

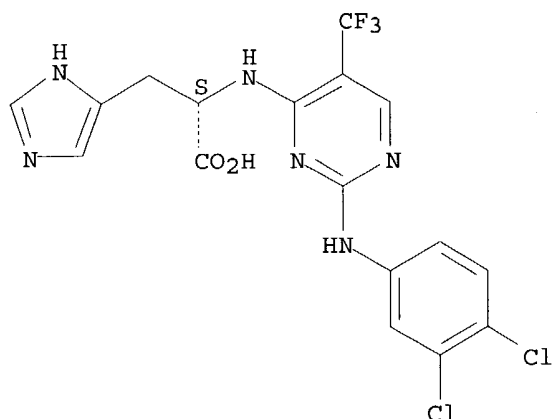
(drug candidate; preparation of trisubstituted pyrimidines as cyclin dependent kinase inhibitors)

RN 514831-25-5 CAPLUS

CN L-Histidine, N-[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

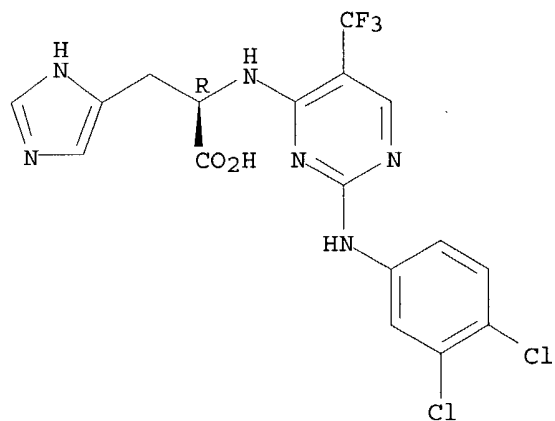
Absolute stereochemistry.

09/ 910,466



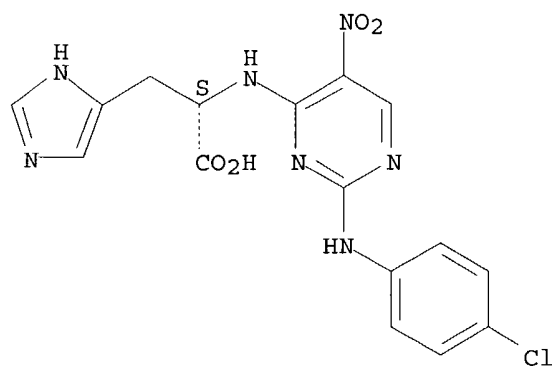
RN 514832-15-6 CAPLUS
CN D-Histidine, N-[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 514832-70-3 CAPLUS
CN L-Histidine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:90023 CAPLUS

DOCUMENT NUMBER: 136:135018

TITLE: Preparation of 3-(heteroaryl) alanine derivatives as

inhibitors of leukocyte adhesion mediated by VLA-4

INVENTOR(S): Konradi, Andrei W.; Pleiss, Michael A.; Thorsett, Eugene D.; Ashwell, Susan; Welmaker, Gregory S.; Kreft, Anthony; Sarantakis, Dimitrios; Dressen, Darren B.; Grant, Francine S.; Semko, Christopher; Xu, Ying-Zi; Stappenbeck, Frank

PATENT ASSIGNEE(S): Elan Pharmaceuticals, Inc., USA; American Home Products Corporation

SOURCE: PCT Int. Appl., 132 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008203	A2	20020131	WO 2001-US23097	20010720
WO 2002008203	A3	20020523		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

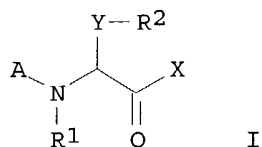
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2002052375	A1	20020502	US 2001-910466	20010719
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PRIORITY APPLN. INFO.: US 2000-220131P P 20000721

OTHER SOURCE(S): MARPAT 136:135018

GI



AB 3-(Heteroaryl)alanine derivs. I [A = an (un)substituted aryl, heteroaryl, cycloalkyl, or heterocyclic group; R2 = a nitrogen containing (un)substituted, heteroaryl; Y = (CH₂)_m; m = 0 or 1; R1 = H, (un)substituted, alkyl, alkenyl, cycloalkyl, cycloalkenyl, aryl, heteroaryl, or heterocyclic; X = OH, (un)substituted alkoxy, alkenoxy, cycloalkoxy, cycloalkenoxo, aryloxy, heteroaryloxy, heterocyclyloxy, or NR₃R₃ [R₃ = H, (un)substituted alkyl, alkenyl, cycloalkyl, aryl, heteroaryl, or heterocyclic]] were prepared as inhibitors of leukocyte adhesion mediated by VLA-4. Compds. I have binding affinity to VLA-4 as expressed by an IC₅₀ of about 15 μM or less. Thus, N-[5-(2,2,2-trifluoroethyl)pyrimidin-4-yl]-DL-3-[5-(2,5-dimethoxyphenyl)pyridin-2-yl]alanine was prepared by multistep procedure via coupling of DL-[5-(2,6-dimethoxyphenyl)pyridine-2-yl]alanine Et ester and 4,6-dichloro-5-(2,2,2-trifluoroethyl)pyrimidine.

IT 392298-39-4P 392298-40-7P 392298-42-9P
392298-43-0P

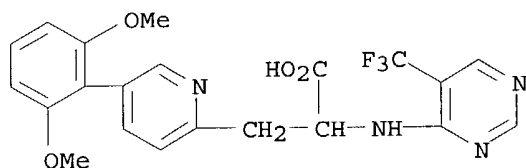
09/ 910,466

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of alanine derivs. as inhibitors of leukocyte adhesion mediated by VLA-4)

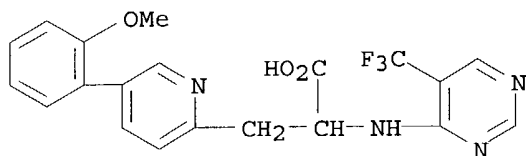
RN 392298-39-4 CAPLUS

CN 2-Pyridinepropanoic acid, 5-(2,6-dimethoxyphenyl)- α -[[5-(trifluoromethyl)-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



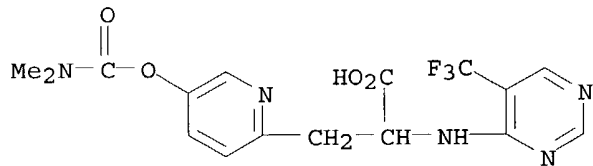
RN 392298-40-7 CAPLUS

CN 2-Pyridinepropanoic acid, 5-(2-methoxyphenyl)- α -[[5-(trifluoromethyl)-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



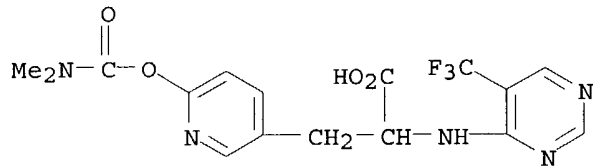
RN 392298-42-9 CAPLUS

CN 2-Pyridinepropanoic acid, 5-[[[(dimethylamino)carbonyl]oxy]- α -[[5-(trifluoromethyl)-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 392298-43-0 CAPLUS

CN 3-Pyridinepropanoic acid, 6-[[[(dimethylamino)carbonyl]oxy]- α -[[5-(trifluoromethyl)-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:63992 CAPLUS

DOCUMENT NUMBER: 134:116237

TITLE: Preparation of bradykinin B1 receptor antagonists

INVENTOR(S): Ohlmeyer, Michael H. J.; Baldwin, John J.; Dolle,

PATENT ASSIGNEE(S): Roland E., III; Paradkar, Vidyadhar; Quintero, Jorge
 SOURCE: Gabriel; Pan, Gonghua
 DOCUMENT TYPE: Pharmacopeia, Inc., USA
 LANGUAGE: PCT Int. Appl., 231 pp.
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION: CODEN: PIXXD2
 Patent
 English

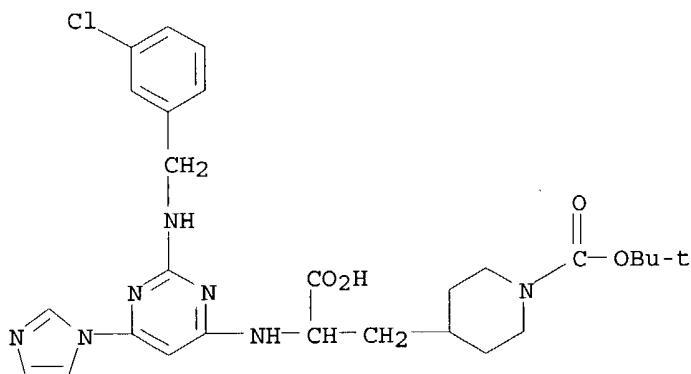
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001005783	A1	20010125	WO 2000-US19185	20000714
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EP 1196411	A1	20020417	EP 2000-950343	20000714
EP 1196411	B1	20030917		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003505384	T2	20030212	JP 2001-511442	20000714
AT 250053	E	20031015	AT 2000-950343	20000714
US 2003229092	A1	20031211	US 2002-46616	20020114
PRIORITY APPLN. INFO.: US 1999-143990P P 19990715 WO 2000-US19185 W 20000714				
OTHER SOURCE(S): MARPAT 134:116237 GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. I [X, Y, Z = CH or N; A = A1 or A2, where A1 is R4R5NCO (R4 = H, aryl, heteroaryl, substituted alkyl; R5 = H, alkyl), 5-aryl-1,2,4-triazol-3-yl, 2-aryl-4-imidazolyl, or 2-aryl-5-thiazolyl and A2 is R7CONH (R7 = aryl or alkylaryl), R7SO2NH, R4NH, R4O; Q = heteroaryl, aryl, CH2R13 (R13 = OH, OTHP, 1-imidazolyl, 1-pyrrolyl), CH:NOMe, or 1,3-dithian-2-yl; W = H, Cl, F, alkyl, aryl, heteroaryl, alkoxy, alkylthio, an amino group, arylcarbonyl, etc.; R1 = alkyl, cycloalkyl, heterocyclyl, aryl, heteroaryl, etc.; R2 = H or alkyl or R1R2C is a ring optionally containing O, S or N; R3 = H or alkyl, or when n is zero, R2 and R3 taken together form a 6-membered ring (with provisos)] were prepared as bradykinin B1 receptor antagonists. Thus, D-leucine derivative II was prepared by substitution reaction of D-leucine 4-chlorobenzylamide with 2,4-dichloro-(or difluoro)-6-(1H-imidazol-1-yl)pyrimidine and then 3-chlorobenzylamine. Pharmaceutical formulations containing II are described.

IT 321328-55-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of bradykinin B1 receptor antagonists)
 RN 321328-55-6 CAPLUS
 CN 4-Piperidinepropanoic acid, α -[[2-[[[(3-chlorophenyl)methyl]amino]-6-(1H-imidazol-1-yl)-4-pyrimidinyl]amino]-1-[(1,1-dimethylethoxy)carbonyl]- (9CI) (CA INDEX NAME)

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REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:508382 CAPLUS

DOCUMENT NUMBER: 119:108382

TITLE: In vitro cytostatic activity of some amino acid 4-N-substituted cytosines

AUTHOR(S): Hladon, Boguslaw; Sloderbach, Anna; Radosh, Przemyslaw; Sychala, Jaroslaw; Golankiewicz, Krzysztof

CORPORATE SOURCE: Dep. Pharmacol., Med. Acad., Poznan, 61-701, Pol. SOURCE: Archivum Immunologiae et Therapiae Experimentalis

(1992), 40(2), 145-50

CODEN: AITEAT; ISSN: 0004-069X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The cytotoxicity of 16 cytosine derivs. substituted at position N4 with amino acid and related moieties was studied on human carcinoma cells in vitro. The activity of the compds. was inversely related to their solubility. The most active compound, and the only one seemed suitable for further investigation, was N4-(1H-2-oxo-4-pyrimidinyl)tryptamine. Some hypothetical structure-activity relationships are briefly discussed.

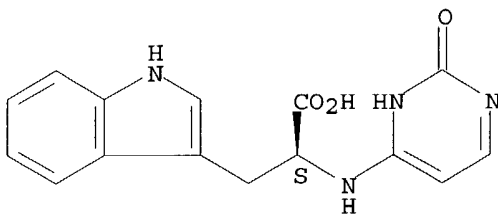
IT 93734-66-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study) (cytostatic activity of, structure in relation to)

RN 93734-66-8 CAPLUS

CN L-Tryptophan, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

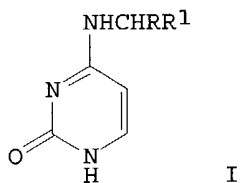
ACCESSION NUMBER: 1989:477735 CAPLUS

DOCUMENT NUMBER: 111:77735

TITLE: Photochemical synthesis of deuterium-labeled 4-N-substituted cytosines

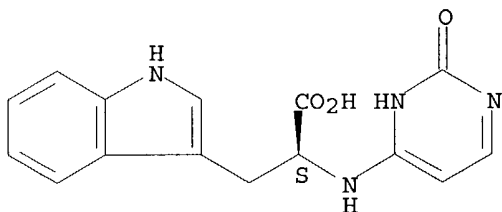
09/ 910,466

AUTHOR(S): Celewicz, Lech; Spychala, Jaroslaw; Golankiewicz, Krzysztof
CORPORATE SOURCE: Fac. Chem., Adam Mickiewicz Univ., Poznan, 60-780, Pol.
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1988), 25(12); 1401-5
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:77735
GI



AB Deuteroalkylcytosines I (R = D; R1 = H, Me, CHMe2, CH2OH, CH2CO2H, CH2Ph, 3-benzimidazolylmethyl) were obtained in 45-85% yield by photochem. decarboxylation of I (R = CO2H) in the presence of D2O or MeOD.
IT 93734-66-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. decarboxylation-deuteration of)
RN 93734-66-8 CAPLUS
CN L-Tryptophan, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:618460 CAPLUS
DOCUMENT NUMBER: 109:218460
TITLE: Intramolecular OH...N .dblharw. O-...H+N hydrogen bonds in N-(1H-2-oxo-4-pyrimidinyl) amino acids
AUTHOR(S): Brzezinski, Bogumil; Celewicz, Lech; Spychala, Jaroslaw; Golankiewicz, Krzysztof
CORPORATE SOURCE: Dep. Chem., Adam Mickiewicz Univ., Poznan, 60-780, Pol.
SOURCE: Chemical Physics Letters (1988), 149(4), 348-54
CODEN: CHPLBC; ISSN: 0009-2614
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Seven N-(1H-2-oxo-4-pyrimidinyl) amino acids were studied by NMR and FTIR spectroscopy. In (CD3)2SO solns. easily polarizable intramol. OH...N .dblharw. O-...H+N bonds were formed and the IR continuum was observed. In aqueous solns. the intramol. H bonds were broken and the tautomeric equilibrium shifted towards the zwitterion.

09/ 910,466

IT 93734-66-8

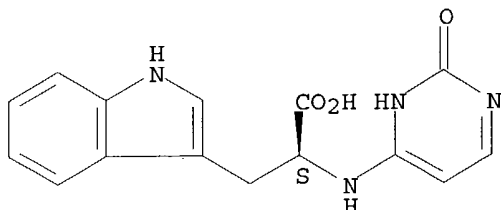
RL: PRP (Properties)

(IR and NMR spectra of, hydrogen bonds in relation to)

RN 93734-66-8 CAPLUS

CN L-Tryptophan, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:610774 CAPLUS

DOCUMENT NUMBER: 109:210774

TITLE: Photochemical synthesis of N4-substituted cytosines
AUTHOR(S): Celewicz, Lech; Sychala, Jaroslaw; Golankiewicz, Krzysztof

CORPORATE SOURCE: Fac. Chem., Adam Mickiewicz Univ., Poznan, 60-780, Pol.

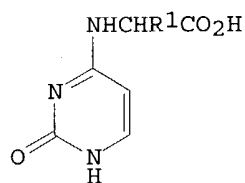
SOURCE: Synthetic Communications (1987), 17(16), 1939-50
CODEN: SYNCAV; ISSN: 0039-7911

DOCUMENT TYPE: Journal

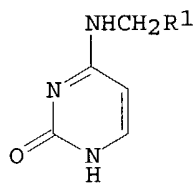
LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:210774

GI



I



II

AB Pyrimidinyl-substituted L-amino acids I [R1 = H, Me, CH2CHMe2, CHMeEt, CH2OH, CH(OH)Me, CH2CO2H, CH2Ph, 3-indolylmethyl] underwent photochem. decarboxylation to give cytosines II. II [R1 = CH2OH, CH(OH)Me] were irradiated to give II (R1 = Me).

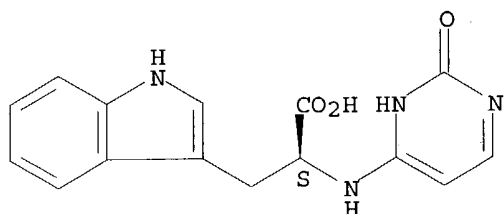
IT 93734-66-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. decarboxylation of)

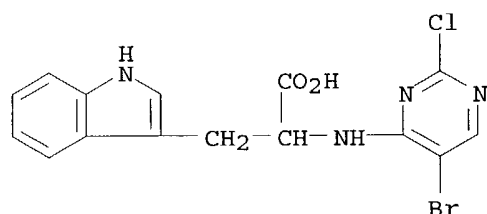
RN 93734-66-8 CAPLUS

CN L-Tryptophan, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1975:422276 CAPLUS
 DOCUMENT NUMBER: 83:22276
 TITLE: Effect of some pyrimidine amino acid derivatives on vaccinia virus in tissue culture
 AUTHOR(S): Izergina, E. A.; Votyakov, V. I.; Balandin, I. G.; Kabailova, I. V.; Seleznev, A. F.; Andreeva, O. T.; Lidak, M. Yu.
 CORPORATE SOURCE: Beloruss. Nauchno-Issled. Inst. Epidemiol., Mikrobiol., Minsk, USSR
 SOURCE: Voprosy Virusologii (1975), (1), 51-4
 CODEN: VVIRAT; ISSN: 0507-4088
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI For diagram(s), see printed CA Issue.
 AB Of the 9 pyrimidine derivs. tested, only N-(2-chloro-5-bromo-4-pyrimidinyl)-DL-leucine (I) [35026-05-2] showed any antiviral activity against vaccinia viruses in chick embryo fibroblast culture. I inhibited DNA synthesis in the infected cultures, and decreased the infectious titer of the virus.
 IT 35023-48-4
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (virus response to, vaccinia)
 RN 35023-48-4 CAPLUS
 CN Tryptophan, N-(5-bromo-2-chloro-4-pyrimidinyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1972:25548 CAPLUS
 DOCUMENT NUMBER: 76:25548
 TITLE: Synthesis of N-(2-chloro-5-bromo-4-pyrimidinyl)- and N-(2-chloro-5-iodo-4-pyrimidinyl)amino acids
 AUTHOR(S): Ulane, I.; Lidaks, M.
 CORPORATE SOURCE: Inst. Org. Sint., Riga, USSR
 SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1971), 7(4), 527-9
 CODEN: KGSSAQ; ISSN: 0132-6244
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian

09/ 910,466

GI For diagram(s), see printed CA Issue.

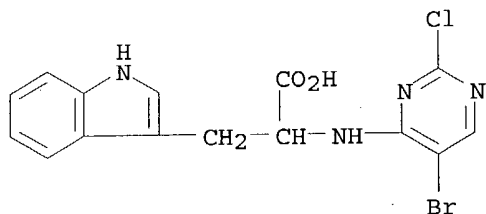
AB The title compds. (I, X = Br, R = DL-NHCHMeCO₂H, DL-leucyl, L-leucyl, L-valyl, DL-methionyl, DL-tryptophanyl, L-isoleucyl, DL-glycyl; and X = I, R = L-leucyl, DL-leucyl, DL-valyl, DL-alanyl) were prepared in 31-50% yield, (from either 2,4-dichloro-5-bromo- or -5-iodopyrimidine and the amino acid Na salt refluxed in H₂O in 1:0.5 molar ratio) for their biol. evaluation as inhibitors of protein biosynthesis.

IT **35023-48-4P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35023-48-4 CAPLUS

CN Tryptophan, N-(5-bromo-2-chloro-4-pyrimidinyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1971:449531 CAPLUS

DOCUMENT NUMBER: 75:49531

TITLE: Synthesis and properties of N-(2-chloro-5-fluoro-4-pyrimidyl)- and N-(2-ethylthio-5-fluoro-4-pyrimidyl) amino acids

AUTHOR(S): Paegle, R.; Plata, M.; Lidaks, M.; Popelis, J.

CORPORATE SOURCE: Inst. Org. Sint., Riga, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1971), 7(2), 258-61

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB The reaction of 2,4-dichloro-5-fluoropyrimidine or 2-(ethylthio)-4-chloro-5-fluoropyrimidine with amino acid sodium salts gave the title compds. (I, R = Cl, EtS; R1 = NHCH₂CO₂H, NHCH(CO₂H)CH₂Ph, NHCH(CO₂H)CH₂CH₂SMe, NHCH(CO₂H)CHMe, NHCH(CO₂H)CH₂CHMe₂, NHCH(CO₂H)CH₂(NC₈H₆, = 3-indolyl) and NHCH₂CH₂CO₂H).

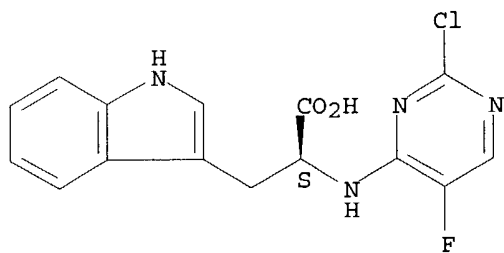
IT **34697-13-7P 34697-14-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 34697-13-7 CAPLUS

CN Tryptophan, N-(2-chloro-5-fluoro-4-pyrimidinyl)-, L- (8CI) (CA INDEX NAME)

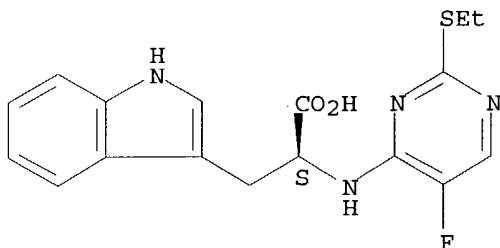
Absolute stereochemistry.



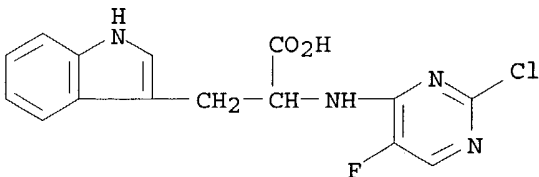
09/ 910,466

RN 34697-14-8 CAPLUS
CN Tryptophan, N-[2-(ethylthio)-5-fluoro-4-pyrimidinyl]-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1966:448006 CAPLUS
DOCUMENT NUMBER: 65:48006
ORIGINAL REFERENCE NO.: 65:9010f-h
TITLE: N-(2-Chloro-5-fluoro-4-pyrimidinyl)amino acids
AUTHOR(S): Paegle, R.; Plata, M.; Lidaks, M.
CORPORATE SOURCE: Inst. Org. Syn., Riga
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1966), (3), 475-6
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB The N-(2-chloro-5-fluoro-4-pyrimidinyl)amino acids (I-VII) obtained from the reaction of 2,4-dichloro-5-fluorouracil with the appropriate amino acids. Me2CHOH-NH4OH-H2O;%, BuOH-HOAc-K2O; R, M.p., Yield, 9:1:1, 4:1:5, 14:1:5; I, H, 169°, 85, 0.87, -, 0.71; II, Me2CH, 179°, 80, -, 0.85, 0.90; III, Me2CHCH2, 173°, 84, -, 0.94, 0.86; IV, MeSCH2CH2, 159°, 66, -, 0.93, 0.81; V, PhCH2, 171°, 79, -, 0.93, 0.80; VI, 182°, 61, -, 0.90, 0.77; VII, 132°, 52, -, 0.88, 0.73;
IT 7662-32-0, Tryptophan, N-(2-chloro-5-fluoro-4-pyrimidinyl)- (preparation of)
RN 7662-32-0 CAPLUS
CN Tryptophan, N-(2-chloro-5-fluoro-4-pyrimidinyl)- (7CI, 8CI) (CA INDEX NAME)



L5 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1966:448005 CAPLUS
DOCUMENT NUMBER: 65:48005
ORIGINAL REFERENCE NO.: 65:9010d-f
TITLE: N-(2-Ethylthio-5-fluoro-4-pyrimidinyl) amino acids
AUTHOR(S): Paegle, R.; Plata, M.; Lidaks, M.
CORPORATE SOURCE: Inst. Org. Syn., Riga

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1966), (3), 474-5
 CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

LANGUAGE: Russian

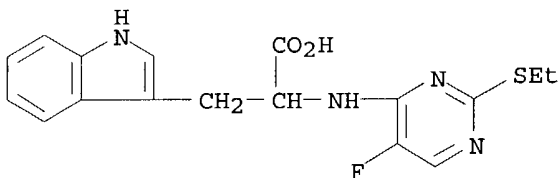
GI For diagram(s), see printed CA Issue.

AB The N-(2-ethylthio-5-fluoro-4-pyrimidinyl)amino acids (I-VII) were obtained from the reaction of 2-ethylthio-4-chloro-5-flourouracil with the appropriate amino acids. Rf; Me2CHOHNH4OHH2O; %, BuOH-HOAc-H2O; R, M.p., Yield, 4:1:5, 9:1:1, 14:1:5; I, H, 215°, 70, -, -, 0.88; II, iso-Pr, 174°, 45, -, 0.85, 0.82; III, iso-Bu, 177°, 73, 0.95, -, 0.86; IV, MeSCH2CH2, 173°, 62, -, 0.84, 0.90; V, PhCH2, 186°, 67, -, 0.85, 0.92; VI, A, 198°, 69, 0.94, -, 0.87; VII, -, 141°, 52, 0.89, -, 0.90;

IT 7662-64-8, Tryptophan, N-[2-(ethylthio)-5-fluoro-4-pyrimidinyl]- (preparation of)

RN 7662-64-8 CAPLUS

CN Tryptophan, N-[2-(ethylthio)-5-fluoro-4-pyrimidinyl]- (7CI, 8CI) (CA INDEX NAME)



L5 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1963:482495 CAPLUS

DOCUMENT NUMBER: 59:82495

ORIGINAL REFERENCE NO.: 59:15376h, 15377a-b

TITLE: Pyrimidine nucleosides. XVII. Pyrimidinyl amino acids

AUTHOR(S): Ueda, Tohru; Fox, Jack J.

CORPORATE SOURCE: Cornell Univ. Med. Coll., New York, NY

SOURCE: Journal of Medicinal Chemistry (1963), 6(6), 697-701 ✓
 CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 59:82495

GI For diagram(s), see printed CA Issue.

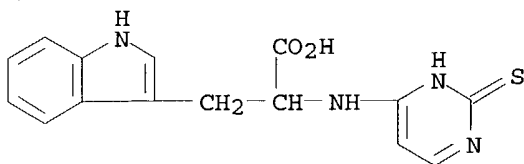
AB cf. CA 58, 11457a. N-(2-Oxo-4-pyrimidinyl) amino acids were prepared by reaction of 4-methylthio-2-pyrimidinones with amino acids. N-(2Oxo-4-pyrimidinyl)glycine, -L-alanine, -L-phenylalanine (I), -L-tryptophan (II), -β-alanine, -o- and p-aminobenzoic acid (III), and -glycylglycine were obtained. N-(2-Thio-4-pyrimidinyl)-L-tryptophan was also prepared as well as the 5-methyl, 5-fluoro (IV), 5-chloro, and 5-bromo analogs of N-(2-oxo-4-pyrimidinyl)-DL-alanine. The ribonucleosides of I, II, and III were synthesized by treatment of 1-β-D-ribofuranosyl-4-methylthio-2-pyrimidinone with the appropriate amino acid. The 1-(2-deoxy-β-D-ribofuranosyl) derivative of IV was synthesized by similar methods. Preliminary results with some of these compds. in exptl. tumors showed no significant antitumor activity. None of the pyrimidinyl amino acids tested supported the growth of certain pyrimidine- or amino acid-requiring mutants of Escherichia coli.

IT 93734-56-6, Tryptophan, N-(1,2-dihydro-2-thioxo-4-pyrimidinyl)-
 93734-66-8, Tryptophan, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- (preparation of)

RN 93734-56-6 CAPLUS

CN Tryptophan, N-(1,2-dihydro-2-thioxo-4-pyrimidinyl)- (7CI) (CA INDEX NAME)

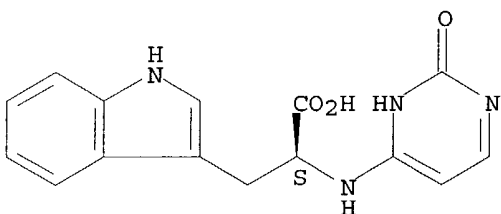
09/ 910,466



RN 93734-66-8 CAPLUS

CN L-Tryptophan, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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FILE 'REGISTRY' ENTERED AT 15:00:20 ON 24 MAR 2004

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L2 STRUCTURE UPLOADED
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L4 16 S L2 FUL

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L5 13 S L4

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